

09/ 422,451

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FILE 'HOME' ENTERED AT 09:11:18 ON 09 FEB 2000

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.15	0.15

FILE 'REGISTRY' ENTERED AT 09:11:26 ON 09 FEB 2000

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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 13, 1999

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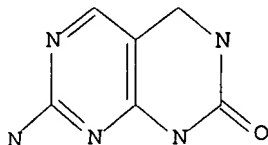
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L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

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Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 09:11:54 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 4 TO ITERATE

100.0% PROCESSED 4 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 4 TO 200

PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s l1 ful

FULL SEARCH INITIATED 09:12:03 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 159 TO ITERATE

100.0% PROCESSED 159 ITERATIONS

72 ANSWERS

SEARCH TIME: 00.00.01

L3 72 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

126.30

126.45

FILE 'CAPLUS' ENTERED AT 09:12:09 ON 09 FEB 2000

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FILE COVERS 1967 - 9 Feb 2000 VOL 132 ISS 7
FILE LAST UPDATED: 8 Feb 2000 (20000208/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s 13

L4 10 L3

=> d 14 1- ibib abs hitstr

YOU HAVE REQUESTED DATA FROM 10 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1999:764041 CAPLUS

DOCUMENT NUMBER: 132:22971

TITLE: Preparation of oxopyrido- and -pyrimidopyrimidines as cellular proliferation inhibitors

INVENTOR(S): Dobrusin, Ellen Myra; Hamby, James Marino; Kramer, James Bernard; Schroeder, Mel Conrad; Showalter, Howard Daniel Hollis; Toogood, Peter; Trumpp-Kallmeyer, Susanne A.

PATENT ASSIGNEE(S): Warner-Lambert Co., USA

SOURCE: PCT Int. Appl., 133 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

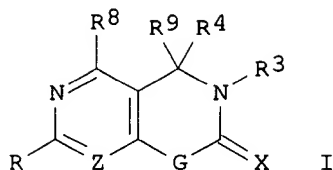
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9961444	A2	19991202	WO 1999-US10187	19990510
W:	AE, AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
PRIORITY APPLN. INFO.:			US 1998-86708	19980526
			US 1999-126158	19990325
OTHER SOURCE(S):	MARPAT 132:22971			

GI



AB Title compds. [I; G = NR₂ or CHR₂; R = NHR₁ or SOO-2R₁; R₁,R₂ = H, (cyclo)alkyl, (un)substituted PH, -pyridyl, etc.; R₃ = groups cited for R₁, OH, alkoxy(carbonyl), etc.; R₄ = H; R₃R₄ = bond; R₈,R₉ = H, halo, NH₂, alkoxy carbonyl, etc.; X = O, S, (alkyl)imino, etc.; Z =N or CH] were prep'd. as cyclin-dependant and tyrosine kinase inhibitors. Thus, 5-aminomethyl-4-cyclopentylamino-2-methylthiopyrimidine (prepn. given) was cyclocondensed with 1,1'-carbonyldiimidazole and the oxidized product aminated by 4-(MeO)C₆H₄NH₂ to give I [G = cyclopentylimino, R = 4-(MeO)C₆H₄NH, R₃ = R₄ = R₈ = R₉ = H, X = O]. Data for biol. activity of I were given.

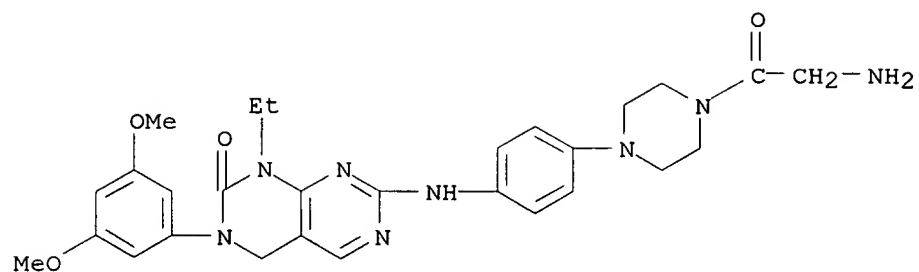
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 251371-90-1P 251371-91-2P 251371-92-3P
 251371-93-4P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of bicyclic pyrimidines and bicyclic 3,4-dihydropyrimidines as inhibitors of cellular proliferation)

RN 251370-13-5 CAPLUS

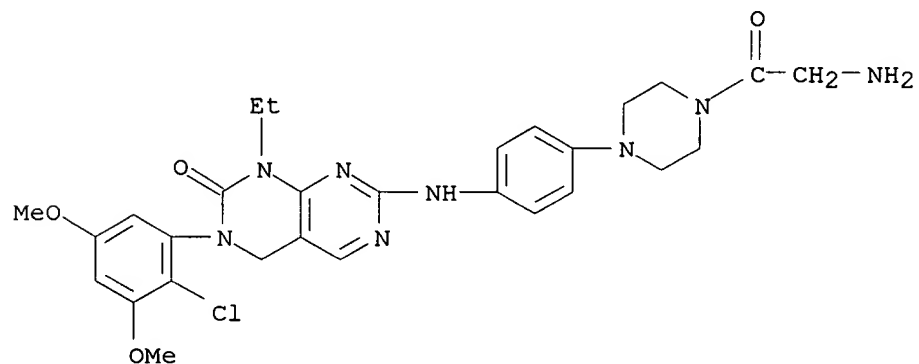
CN Piperazine,

1-(aminoacetyl)-4-[4-[[6-(3,5-dimethoxyphenyl)-8-ethyl-5,6,7,8-tetrahydro-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]phenyl]- (9CI) (CA INDEX NAME)



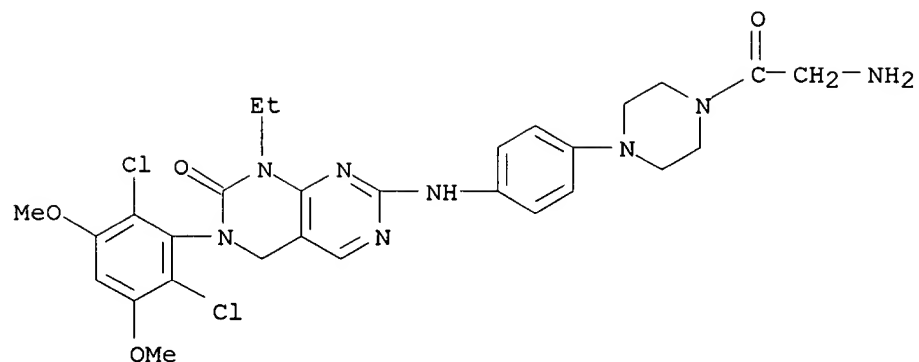
RN 251370-14-6 CAPLUS

CN Piperazine, 1-(aminoacetyl)-4-[4-[[6-(2-chloro-3,5-dimethoxyphenyl)-8-ethyl-5,6,7,8-tetrahydro-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]phenyl]-(9CI) (CA INDEX NAME)



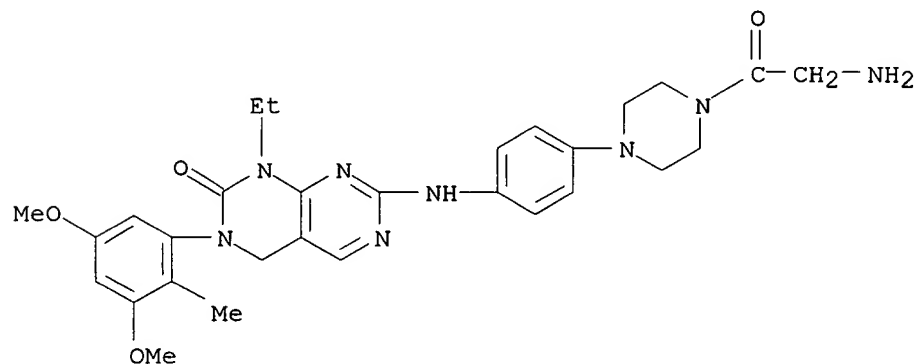
RN 251370-15-7 CAPLUS

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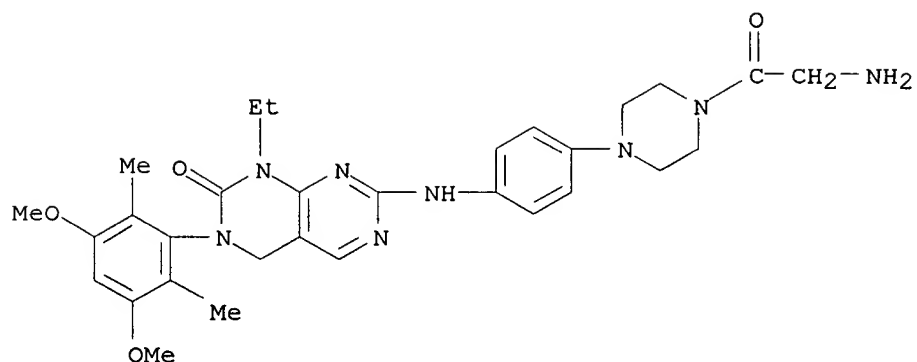
RN 251370-16-8 CAPLUS

CN Piperazine, 1-(aminoacetyl)-4-[4-[[6-(3,5-dimethoxy-2-methylphenyl)-8-ethyl-5,6,7,8-tetrahydro-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]phenyl]-(9CI) (CA INDEX NAME)



RN 251370-17-9 CAPLUS

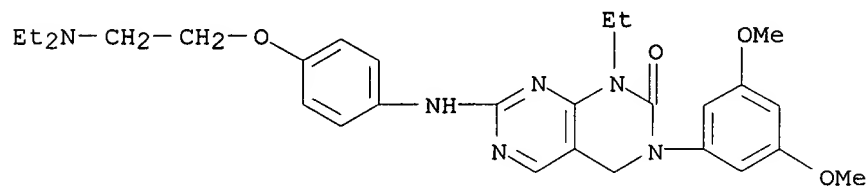
CN Piperazine, 1-(aminoacetyl)-4-[4-[[6-(3,5-dimethoxy-2,6-dimethylphenyl)-8-ethyl-5,6,7,8-tetrahydro-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]phenyl]-(9CI) (CA INDEX NAME)



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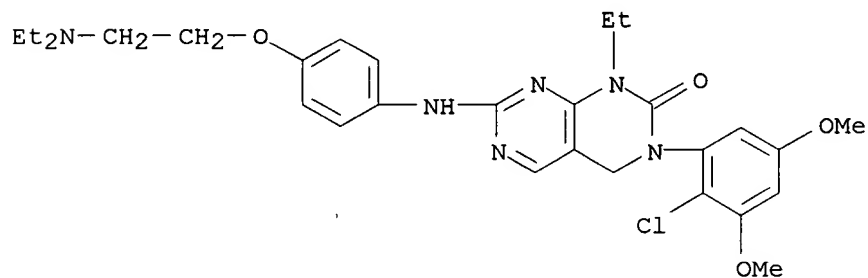
7-[[4-[2-(diethylamino)ethoxy]phenyl]amino]-3-(3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)



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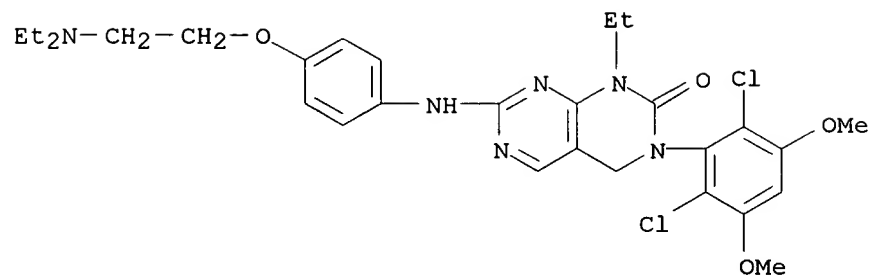
3-(2-chloro-3,5-dimethoxyphenyl)-7-[[4-[2-(diethylamino)ethoxy]phenyl]amino]-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)



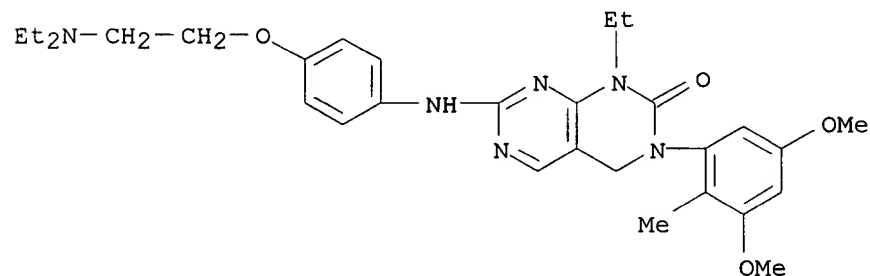
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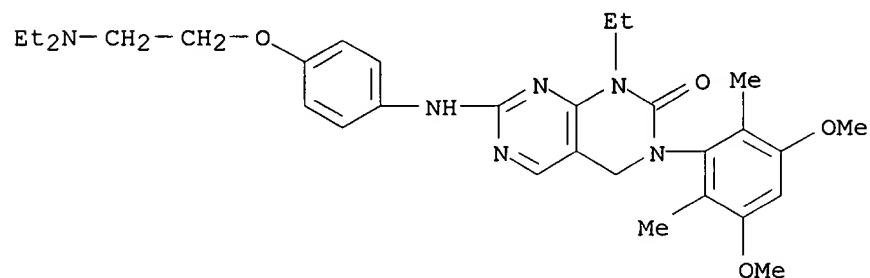
3-(2,6-dichloro-3,5-dimethoxyphenyl)-7-[[4-[2-(diethylamino)ethoxy]phenyl]amino]-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)



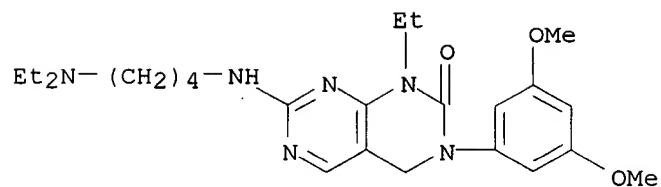
RN 251370-21-5 CAPLUS
 CN Pyrimido[4,5-d]pyrimidin-2(1H)-one,
 7-[[4-[2-(diethylamino)ethoxy]phenyl]a
 mino]-3-(3,5-dimethoxy-2-methylphenyl)-1-ethyl-3,4-dihydro- (9CI) (CA
 INDEX NAME)



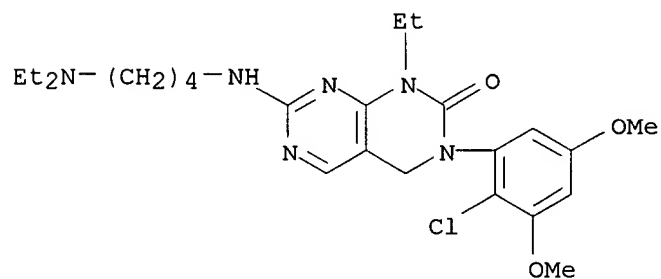
RN 251370-22-6 CAPLUS
 CN Pyrimido[4,5-d]pyrimidin-2(1H)-one,
 7-[[4-[2-(diethylamino)ethoxy]phenyl]a
 mino]-3-(3,5-dimethoxy-2,6-dimethylphenyl)-1-ethyl-3,4-dihydro- (9CI)
 (CA
 INDEX NAME)



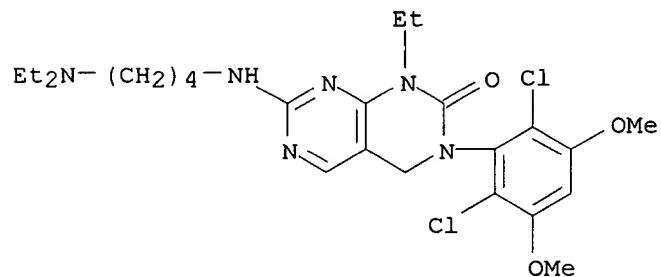
RN 251370-23-7 CAPLUS
 CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 7-[[4-(diethylamino)butyl]amino]-3-
 (3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)



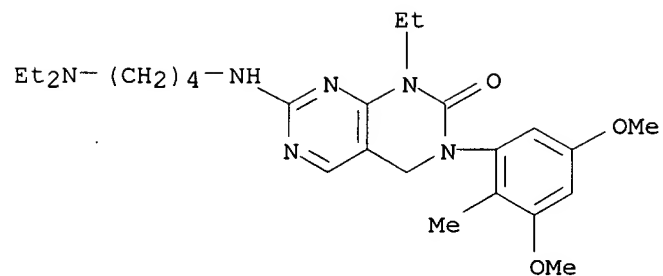
RN 251370-24-8 CAPLUS
 CN Pyrimido[4,5-d]pyrimidin-2(1H)-one,
 3-(2-chloro-3,5-dimethoxyphenyl)-7-[[4-(diethylamino)butyl]amino]-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)



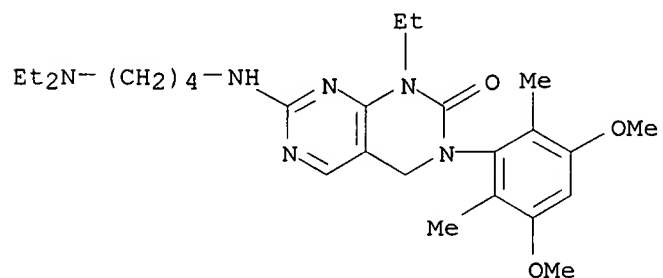
RN 251370-25-9 CAPLUS
 CN Pyrimido[4,5-d]pyrimidin-2(1H)-one,
 3-(2,6-dichloro-3,5-dimethoxyphenyl)-7-[[4-(diethylamino)butyl]amino]-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)



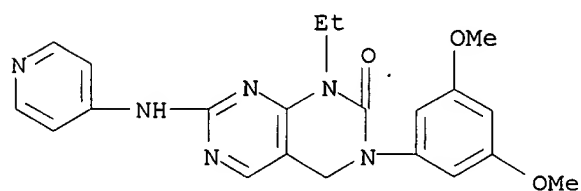
RN 251370-26-0 CAPLUS
 CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 7-[[4-(diethylamino)butyl]amino]-3-(3,5-dimethoxy-2-methylphenyl)-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)



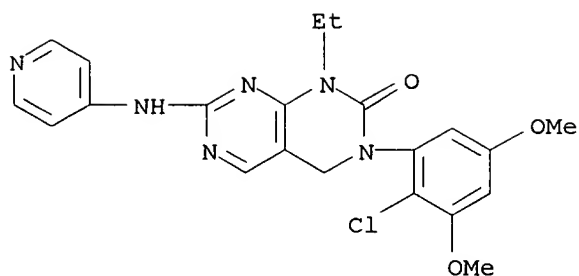
RN 251370-27-1 CAPLUS
 CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 7-[[4-(diethylamino)butyl]amino]-3-(3,5-dimethoxy-2,6-dimethylphenyl)-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)



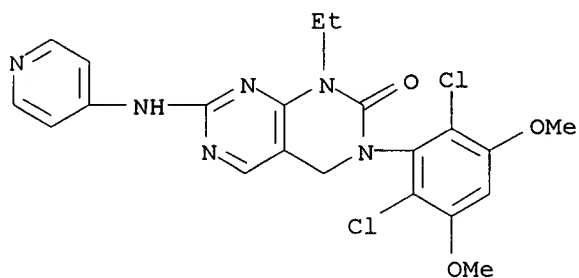
RN 251370-28-2 CAPLUS
 CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro-7-(4-pyridinylamino)- (9CI) (CA INDEX NAME)



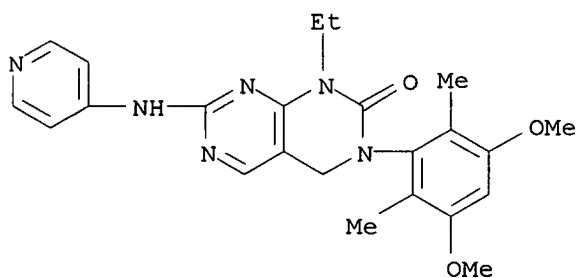
RN 251370-29-3 CAPLUS
 CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(2-chloro-3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro-7-(4-pyridinylamino)- (9CI) (CA INDEX NAME)



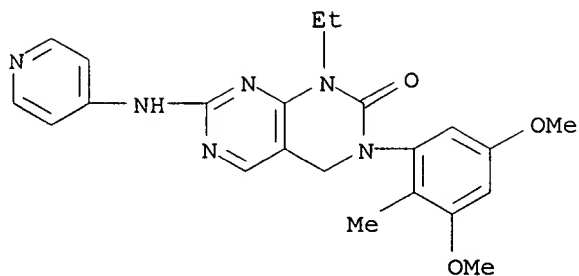
RN 251370-30-6 CAPLUS
 CN Pyrimido[4,5-d]pyrimidin-2(1H)-one,
 3-(2,6-dichloro-3,5-dimethoxyphenyl)-1-
 ethyl-3,4-dihydro-7-(4-pyridinylamino)- (9CI) (CA INDEX NAME)



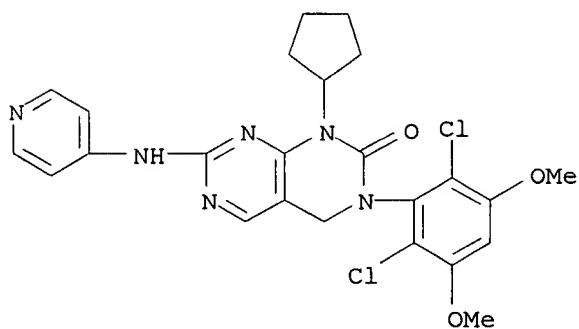
RN 251370-31-7 CAPLUS
 CN Pyrimido[4,5-d]pyrimidin-2(1H)-one,
 3-(3,5-dimethoxy-2,6-dimethylphenyl)-1-
 ethyl-3,4-dihydro-7-(4-pyridinylamino)- (9CI) (CA INDEX NAME)



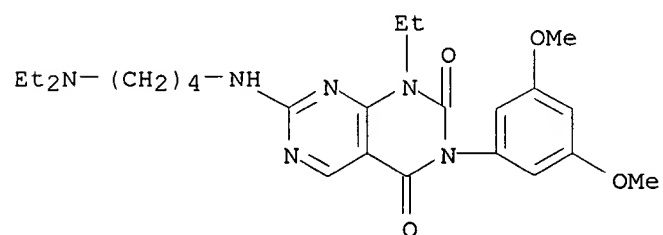
RN 251370-32-8 CAPLUS
 CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(3,5-dimethoxy-2-methylphenyl)-1-
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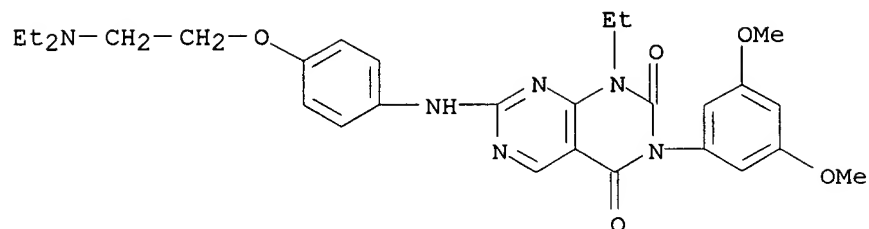
RN 251370-33-9 CAPLUS
 CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 1-cyclopentyl-3-(2,6-dichloro-3,5-dimethoxyphenyl)-3,4-dihydro-7-(4-pyridinylamino)- (9CI) (CA INDEX NAME)



RN 251370-66-8 CAPLUS
 CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-[[4-(diethylamino)butyl]amino]-3-(3,5-dimethoxyphenyl)-1-ethyl- (9CI) (CA INDEX NAME)

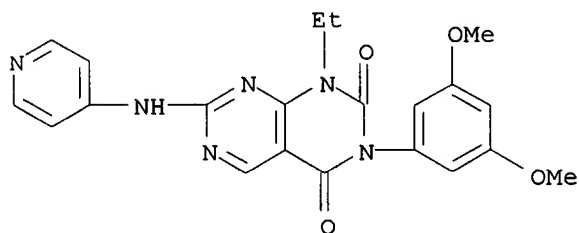


RN 251370-67-9 CAPLUS
 CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-[[4-[2-(diethylamino)ethoxy]phenyl]amino]-3-(3,5-dimethoxyphenyl)-1-ethyl- (9CI) (CA INDEX NAME)



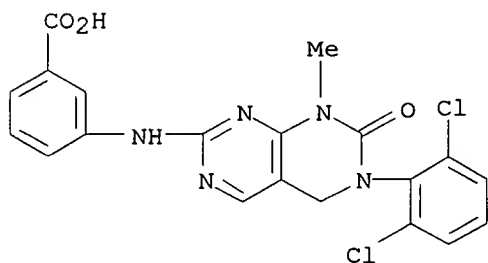
RN 251370-68-0 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 3-(3,5-dimethoxyphenyl)-1-ethyl-7-(4-pyridinylamino)- (9CI) (CA INDEX NAME)



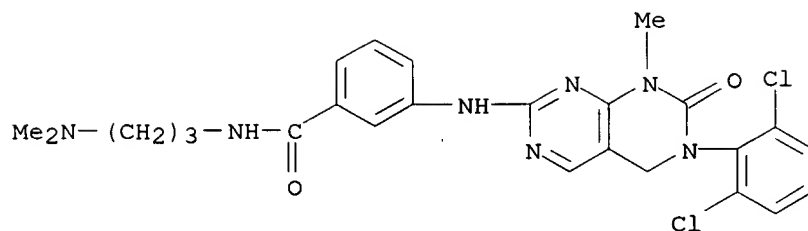
RN 251371-07-0 CAPLUS

CN Benzoic acid, 3-[[6-(2,6-dichlorophenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)



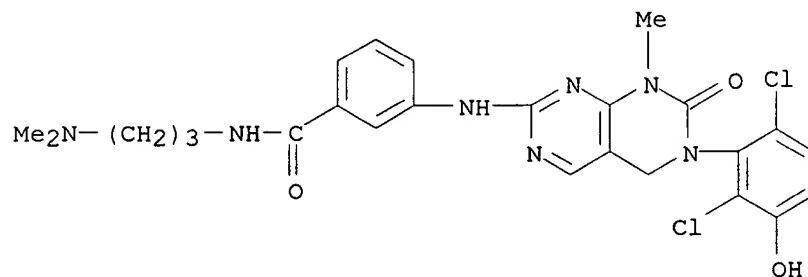
RN 251371-08-1 CAPLUS

CN Benzamide, 3-[[6-(2,6-dichlorophenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]-N-[3-(dimethylamino)propyl]- (9CI)
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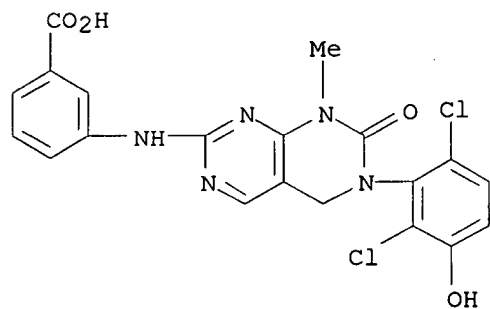
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CN Benzamide, 3-[[6-(2,6-dichloro-3-hydroxyphenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]-N-[3-(dimethylamino)propyl]- (9CI) (CA INDEX NAME)



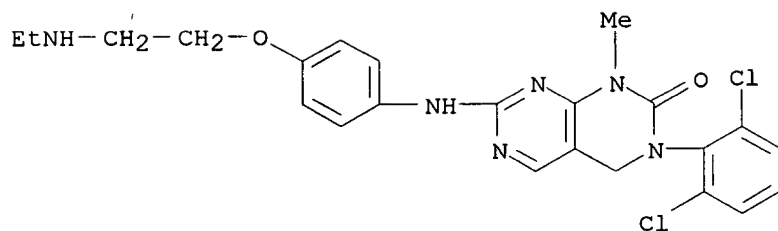
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CN Benzoic acid, 3-[[6-(2,6-dichloro-3-hydroxyphenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)

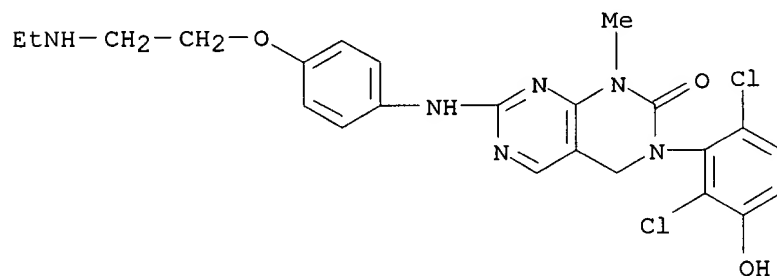


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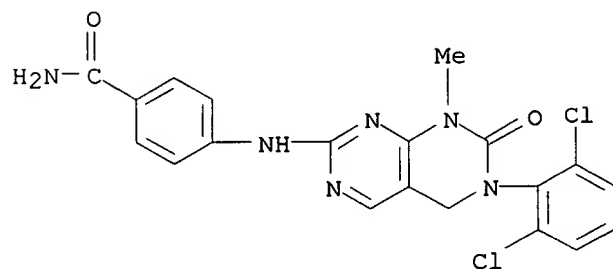
CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(2,6-dichlorophenyl)-7-[[4-[2-(ethylamino)ethoxy]phenyl]amino]-3,4-dihydro-1-methyl- (9CI) (CA INDEX NAME)



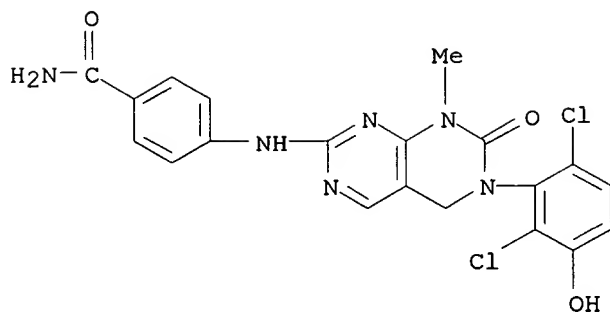
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 INDEX
 NAME)



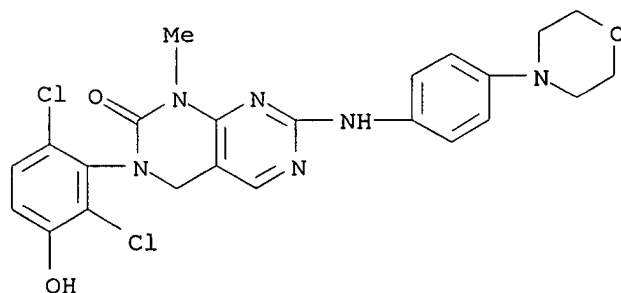
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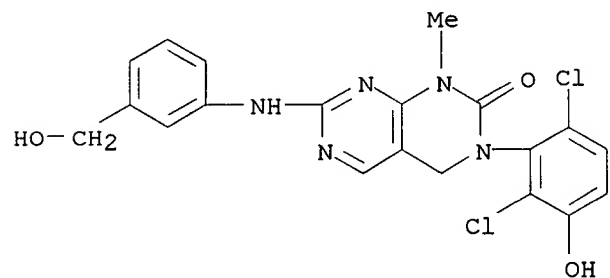
RN 251371-14-9 CAPLUS
 CN Benzamide, 4-[[6-(2,6-dichloro-3-hydroxyphenyl)-5,6,7,8-tetrahydro-8-
 methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)



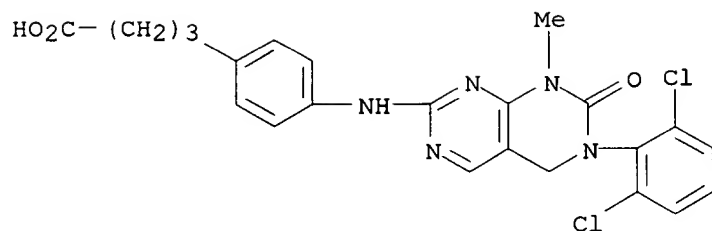
RN 251371-17-2 CAPLUS
 CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(2,6-dichloro-3-hydroxyphenyl)-3,4-dihydro-1-methyl-7-[[4-(4-morpholinyl)phenyl]amino]- (9CI) (CA INDEX NAME)



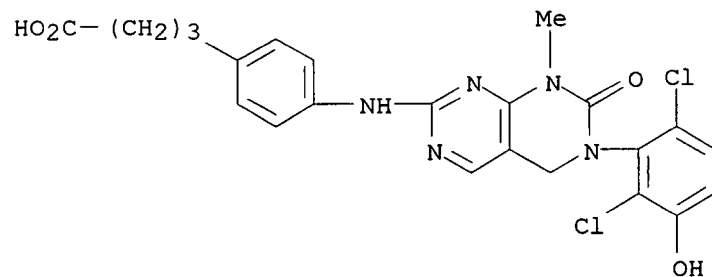
RN 251371-18-3 CAPLUS
 CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(2,6-dichloro-3-hydroxyphenyl)-3,4-dihydro-7-[[3-(hydroxymethyl)phenyl]amino]-1-methyl- (9CI) (CA INDEX NAME)



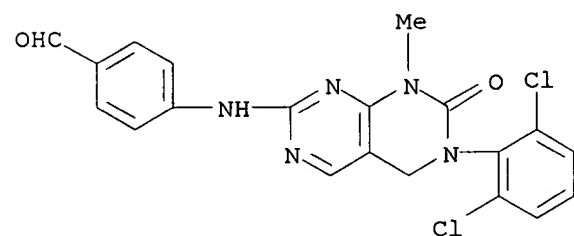
RN 251371-19-4 CAPLUS
 CN Benzenebutanoic acid, 4-[[6-(2,6-dichlorophenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)



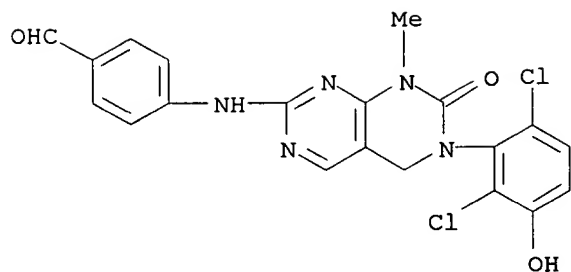
RN 251371-20-7 CAPLUS
 CN Benzenebutanoic acid, 4-[[6-(2,6-dichloro-3-hydroxyphenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)



RN 251371-21-8 CAPLUS
 CN Benzaldehyde, 4-[[6-(2,6-dichlorophenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)

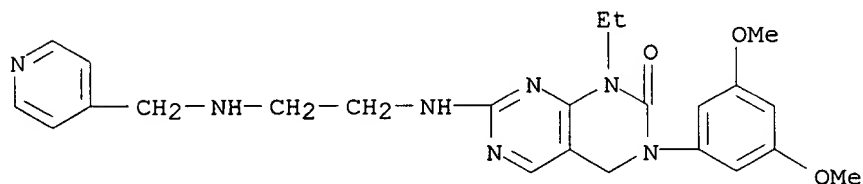


RN 251371-22-9 CAPLUS
 CN Benzaldehyde, 4-[[6-(2,6-dichloro-3-hydroxyphenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)



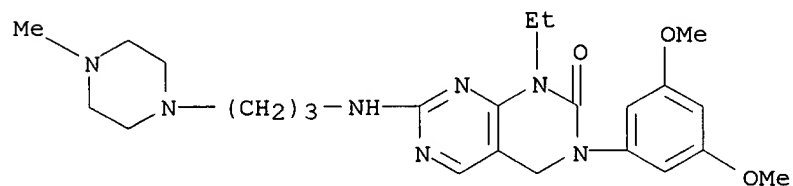
RN 251371-89-8 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro-7-[[2-[(4-pyridinylmethyl)amino]ethyl]amino]- (9CI) (CA INDEX NAME)



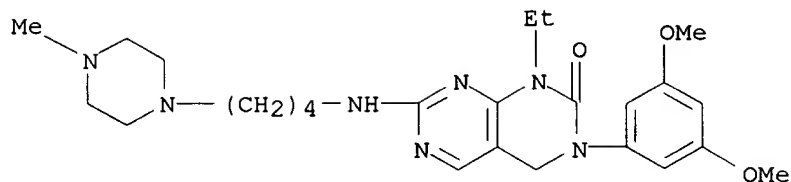
RN 251371-90-1 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro-7-[[3-(4-methyl-1-piperazinyl)propyl]amino]- (9CI) (CA INDEX NAME)



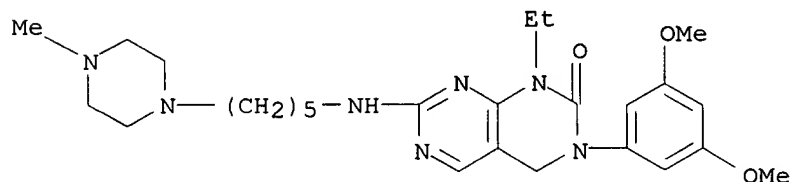
RN 251371-91-2 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro-7-[[4-(4-methyl-1-piperazinyl)butyl]amino]- (9CI) (CA INDEX NAME)



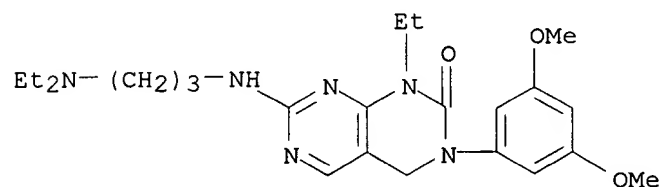
RN 251371-92-3 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro-7-[[5-(4-methyl-1-piperazinyl)pentyl]amino]- (9CI) (CA INDEX NAME)



RN 251371-93-4 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 7-[[3-(diethylamino)propyl]amino]-3-(3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)

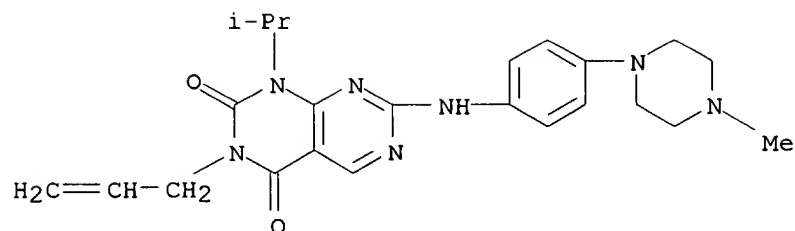


IT 251372-02-8P 251372-03-9P 251372-04-0P
251372-05-1P

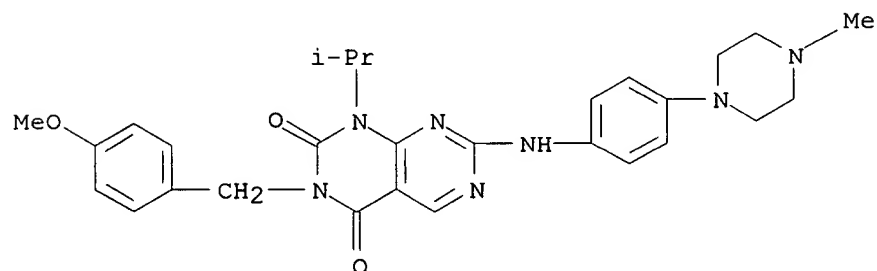
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of bicyclic pyrimidines and bicyclic 3,4-dihydropyrimidines as inhibitors of cellular proliferation)

RN 251372-02-8 CAPLUS

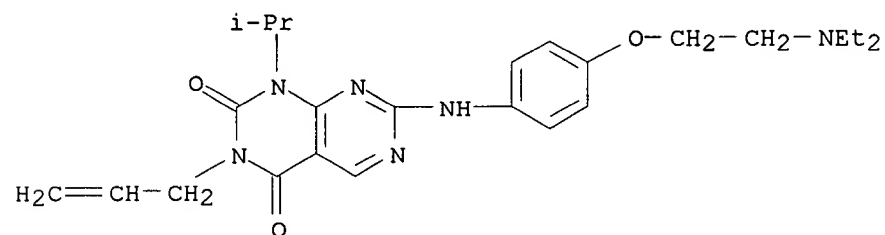
CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 1-(1-methylethyl)-7-[[4-(4-methyl-1-piperazinyl)phenyl]amino]-3-(2-propenyl)- (9CI) (CA INDEX NAME)



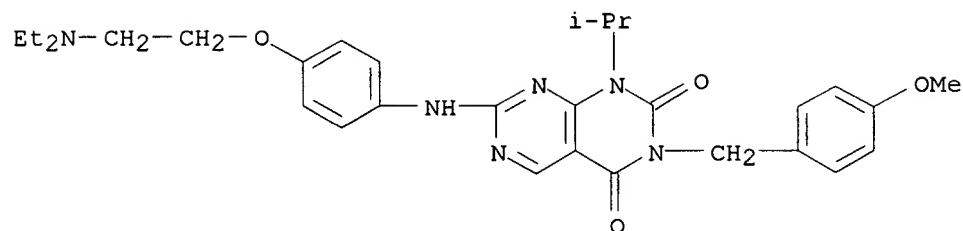
RN 251372-03-9 CAPLUS
 CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione,
 3-[(4-methoxyphenyl)methyl]-1-
 (1-methylethyl)-7-[[4-(4-methyl-1-piperazinyl)phenyl]amino]- (9CI) (CA
 INDEX NAME)



RN 251372-04-0 CAPLUS
 CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-[[4-[2-
 (diethylamino)ethoxy]phenyl]amino]-1-(1-methylethyl)-3-(2-propenyl)-
 (9CI)
 (CA INDEX NAME)



RN 251372-05-1 CAPLUS
 CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-[[4-[2-
 (diethylamino)ethoxy]phenyl]amino]-3-[(4-methoxyphenyl)methyl]-1-(1-
 methylethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1995:334056 CAPLUS

DOCUMENT NUMBER: 122:239631

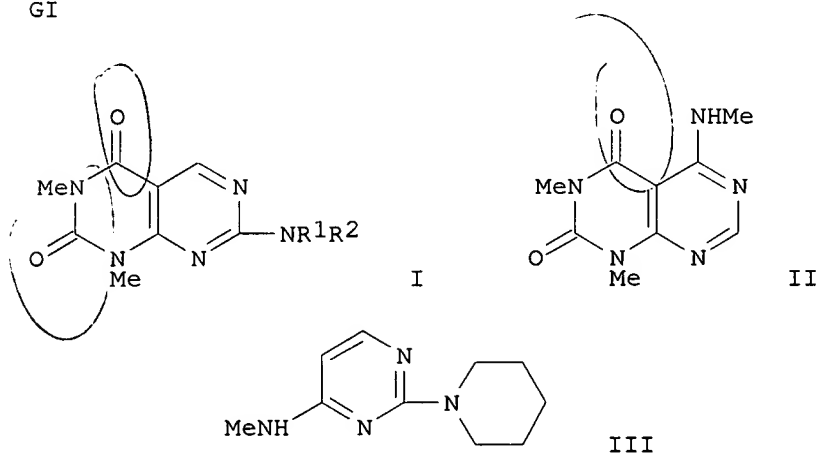
TITLE: Purines, pyrimidines and condensed systems based on them. 12. 1,3-Dimethylpyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione: the first case of regioselective amination of condensed pyrimidines at position 2
Gulevskaya, A. V.; Pozharsky, A. F.; Shorshnev, S. V.;

AUTHOR(S): Zheltushkina, E. A.
CORPORATE SOURCE: Rostov. Gos. Univ., Rostov-on-Don, 344006, Russia
SOURCE: Khim. Geterotsikl. Soedin. (1994), (9), 1249-52
CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI



AB Amination of the title compd. in the presence of an oxidizing agent gave 7-amino derivs. (I; NR1R2 = NH2, NHMe, NHEt, NHCMe3, piperidino, morpholino); in the case of Me2NH the 4-substituted deriv. (II) was also formed. Successive hydrolysis of I (NR1R2 = piperidino) in alk. and acidic medium gave 4-(methylamino)-2-piperidinopyrimidine (III).

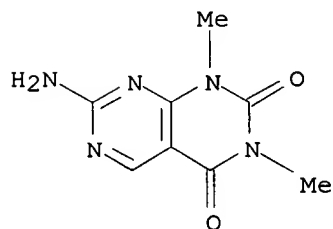
IT 94839-44-8P 94839-45-9P 162147-58-2P

162147-59-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

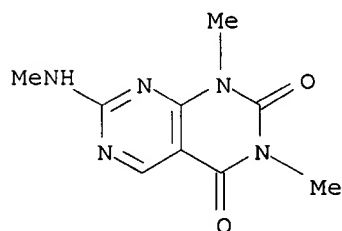
RN 94839-44-8 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-1,3-dimethyl- (9CI)
(CA INDEX NAME)



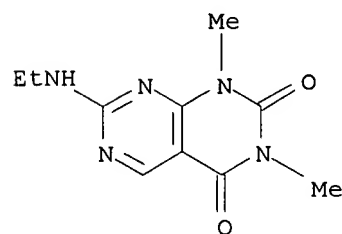
RN 94839-45-9 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 1,3-dimethyl-7-(methylamino)- (9CI) (CA INDEX NAME)



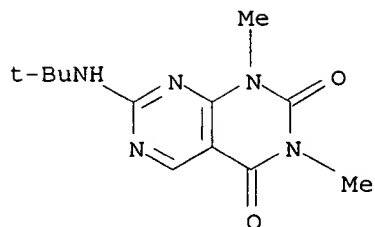
RN 162147-58-2 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-(ethylamino)-1,3-dimethyl- (9CI) (CA INDEX NAME)

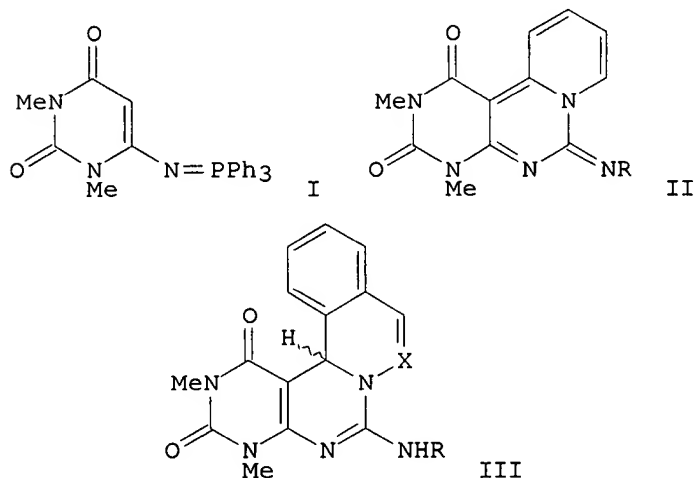


RN 162147-59-3 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-[(1,1-dimethylethyl)amino]-1,3-dimethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1994:134411 CAPLUS
 DOCUMENT NUMBER: 120:134411
 TITLE: Reactions of uracils. 21. Zwitterionic heteropolycyclic uracils by a novel three-component reaction: iminophosphorane, isocyanate, heteroarene
 AUTHOR(S): Wamhoff, Heinrich; Schmidt, Andreas
 CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, D-53121, Germany
 SOURCE: J. Org. Chem. (1993), 58(25), 6976-84
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 120:134411
 GI



AB The novel three-component reaction of (uracil-6-ylimino)phosphorane I, isocyanate, and (substituted) pyridines gives, in a one-pot procedure, a variety of new pyrido[1',2':3,4]pyrimido[4,5-d]pyrimidines, e.g., II (R = aryl, Me₂CH, tosyl, allyl). The zwitterionic ground state of these new ring systems is established by solvatochromism, Hammett correlations, NMR, and X-ray anal. Replacement of the pyridine by isoquinoline and

phthalazine gives access to the novel ring systems
 pyrimido[4',5':4,5]pyrimido[6,1-a]isoquinoline and -phthalazine, which
 are formed as dihydro derivs. [III; X = CH, N (15); R = aryl] or as
 zwitterions, depending on the reaction conditions. Oxidative cleavage of
 the phthalazine 15 in nitrobenzene affords the (cyanophenyl)pyrimido[4,5-
 d]pyrimidines.

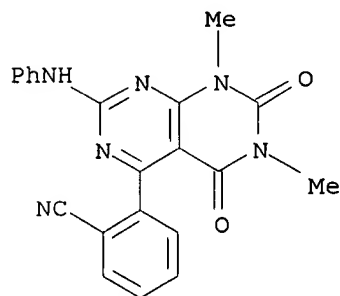
IT 152897-89-7P 152897-90-0P 152897-91-1P

152897-92-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and oxidn. or thermal cleavage of)

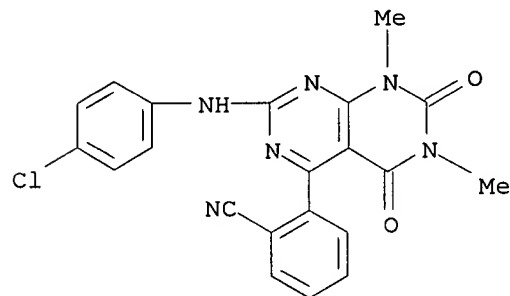
RN 152897-89-7 CAPLUS

CN Benzonitrile, 2-[5,6,7,8-tetrahydro-6,8-dimethyl-5,7-dioxo-2-
 (phenylamino)pyrimido[4,5-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)



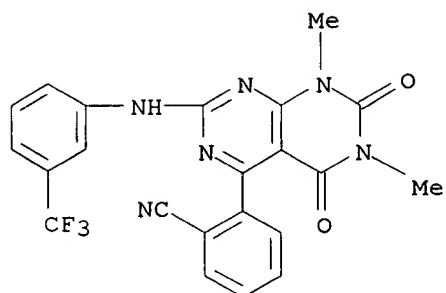
RN 152897-90-0 CAPLUS

CN Benzonitrile, 2-[2-[(4-chlorophenyl)amino]-5,6,7,8-tetrahydro-6,8-dimethyl-
 5,7-dioxopyrimido[4,5-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

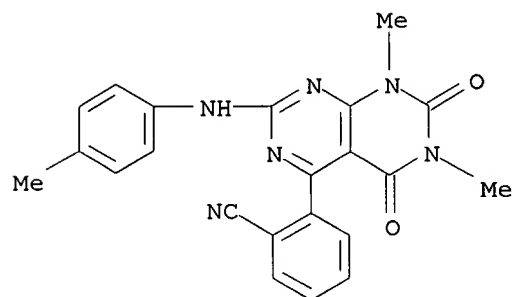


RN 152897-91-1 CAPLUS

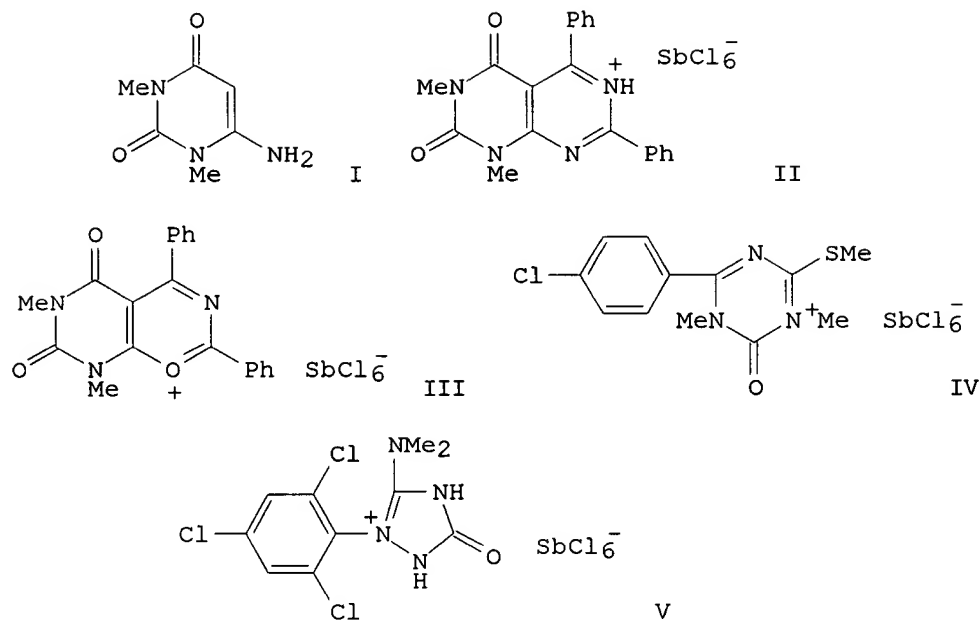
CN Benzonitrile, 2-[5,6,7,8-tetrahydro-6,8-dimethyl-5,7-dioxo-2-[[3-
 (trifluoromethyl)phenyl]amino]pyrimido[4,5-d]pyrimidin-4-yl]- (9CI) (CA
 INDEX NAME)



RN 152897-92-2 CAPLUS
 CN Benzonitrile,
 2-[5,6,7,8-tetrahydro-6,8-dimethyl-2-[(4-methylphenyl)amino]-
 5,7-dioxopyrimido[4,5-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1992:531144 CAPLUS
 DOCUMENT NUMBER: 117:131144
 TITLE: Cyclization reactions of chloro-substituted
 2-azoniaallene salts with bifunctional nucleophiles
 AUTHOR(S): Hamed, Atef
 CORPORATE SOURCE: Fac. Sci., Menoufia Univ., Shebin El-Koom, Egypt
 SOURCE: Synthesis (1992), (6), 591-5
 CODEN: SYNTBF; ISSN: 0039-7881
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Multifunctional electrophilic chloro-substituted 2-azoniaallene salts react with bifunctional nucleophiles to furnish heterocycles. Thus, $\text{PhCCl:N}^+:\text{CClPh SbCl}_6^-$ reacts with pyrimidinedione I to give pyrimidopyrimidinedione salt II. Pyrimido-1,3-oxazin-1-ium salts, e.g., III, representing a new ring system, triazininium salts, e.g., IV, and a triazolium salt (V) are also obtained.

IT **143249-47-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

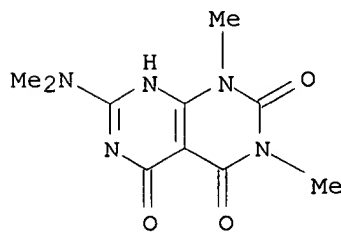
RN 143249-47-2 CAPLUS

CN Antimonate(1-), hexachloro-, (OC-6-11)-, hydrogen, compd. with
7-(dimethylamino)-1,3-dimethylpyrimido[4,5-d]pyrimidine-2,4,5(1H,3H,6H)-
trione (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 143249-46-1

CMF C10 H13 N5 O3



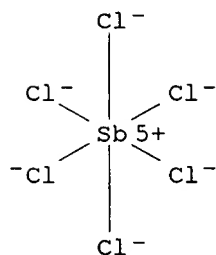
CM 2

CRN 16941-91-6

CMF Cl6 Sb . H

CCI CCS

CDES 7:OC-6-11

● H⁺

L4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1990:514913 CAPLUS

DOCUMENT NUMBER: 113:114913

TITLE: Pyrimidines. 63. Novel ring transformations of
5-cyanouracils into 2-thiocytosines,
2,4-diaminopyrimidines, and

pyrimido[4,5-d]pyrimidines

by the reaction with thioureas and guanidines

AUTHOR(S): Hirota, Kosaku; Sajiki, Hironao; Kitade, Yukio; Maki,
Yoshifumi

CORPORATE SOURCE: Gifu Pharm. Univ., Gifu, 502, Japan

SOURCE: J. Chem. Soc., Perkin Trans. 1 (1990), (1), 123-8

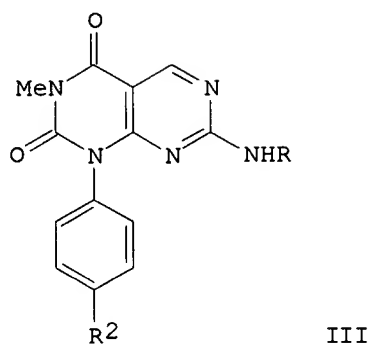
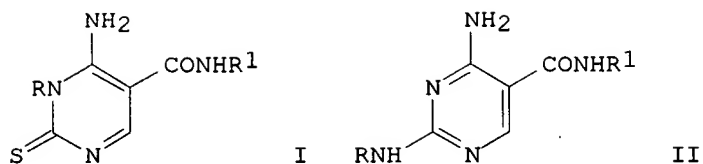
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:114913

GI



AB 1,3-Disubstituted 5-cyanouracils react with thioureas and guanidines to give the 5-carbamoyl-2-thiocytosines I (R = H, Me, Bu, Ph; R1 = Me, cyclohexyl) and 2,4-diamino-5-carbamoylpyrimidines II (R = Ph, Me; R1 = Me, H), resp. On the other hand, 1-aryl-5-cyanouracils react with thioureas to give 7-aminopyrimido [4,5-d]pyrimidine-2,4-diones III (R = H,

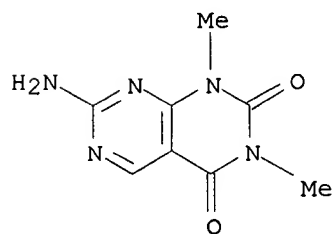
Me; R2 H, OMe).

IT **94839-44-8P 101989-67-7P 128836-42-0P**
129088-65-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

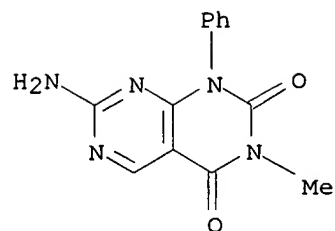
RN 94839-44-8 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-1,3-dimethyl- (9CI)
 (CA INDEX NAME)

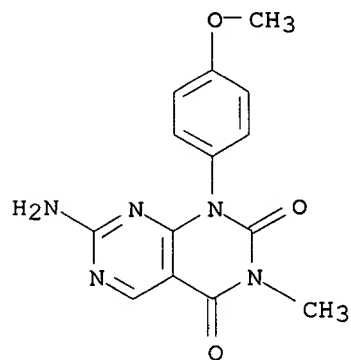


RN 101989-67-7 CAPLUS

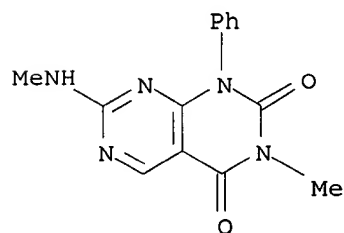
CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-3-methyl-1-phenyl- (9CI)
 (CA INDEX NAME)



RN 128836-42-0 CAPLUS
 CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione,
 7-amino-1-(4-methoxyphenyl)-3-
 methyl- (9CI) (CA INDEX NAME)



RN 129088-65-9 CAPLUS
 CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 3-methyl-7-(methylanilino)-1-
 phenyl- (9CI) (CA INDEX NAME)

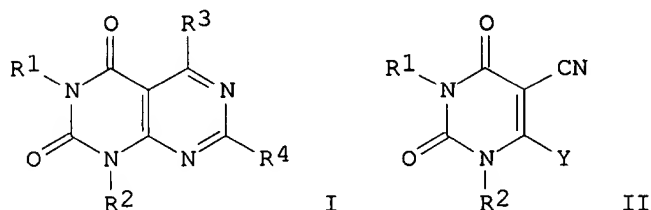


L4 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1987:162576 CAPLUS
 DOCUMENT NUMBER: 106:162576
 TITLE: Preparation and formulations of pyrimido[4,5-
 d]pyrimidine derivatives as antiallergics
 INVENTOR(S): Kitamura, Norihiko; Onishi, Akimoto
 PATENT ASSIGNEE(S): Nippon Zoki Pharmaceutical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

DOCUMENT TYPE: CODEN: JKXXAF
 Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61249988	A2	19861107	JP 1985-90357	19850425
JP 06013518	B4	19940223		

GI



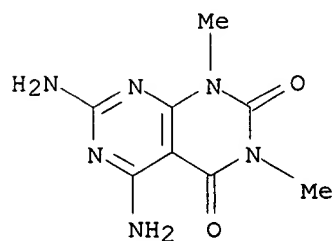
AB The title compds. (I; R1, R2 = alkyl; R3 = NH2, alkylamino; R4 = H, alkyl, Ph, NH2) are prepd. from uracil derivs. (I; R1 and R2 = alkyl; Y = NH2, halo, dialkylaminomethyleneamino) and H2NZ (Z = C:XR4; X = O, NH; R4 = H, alkyl, Ph, NH2). Thus, 6-amino-5-cyano-1,3-dimethyluracil was cyclized with formamide to give 5-amino-1,3-dimethylpyrimido[4,5-d]pyrimidine-2,4-dione (III). III at 100 mg/kg in rats inhibited allergic reactions. A tablet contained III 10, lactose 130, starch 40, and Mg stearate 10 mg.

IT 56007-62-6P

RL: PREP (Preparation)
 (prepn. of, as antiallergic)

RN 56007-62-6 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 5,7-diamino-1,3-dimethyl-
 (9CI) (CA INDEX NAME)



L4 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1986:186439 CAPLUS

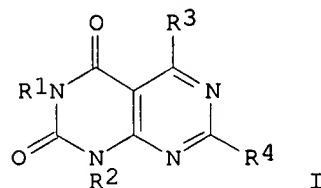
DOCUMENT NUMBER: 104:186439

TITLE: Pyrimidopyrimidinedione derivatives and their use as
 anti-allergic agents

INVENTOR(S): Kitamura, Norihiko; Ohnishi, Akimoto
 PATENT ASSIGNEE(S): Nippon Zoki Pharmaceutical Co., Ltd., Japan
 SOURCE: Eur. Pat. Appl., 51 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 163599	A2	19851204	EP 1985-810182	19850424
EP 163599	A3	19870225		
EP 163599	B1	19900321		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 60226882	A2	19851112	JP 1984-83557	19840424
JP 05059118	B4	19930830		
AT 51231	E	19900415	AT 1985-810182	19850424
US 4886807	A	19891212	US 1988-277447	19881129
PRIORITY APPLN. INFO.:			JP 1984-83557	19840424
			EP 1985-810182	19850424
			US 1985-726618	19850424

GI



AB The title compds. (I; R1 = alkyl; R2 = alkyl, Ph; R3 = H, alkyl, alkylamino; R4 = H, (halo)alkyl, Ph, amino, alkylamino) were prepd.

Thus,

6-amino-1,3-dimethyluracil underwent Vilsmeier reaction with HCONMe₂ to give 95% 5-[(dimethylamino)methylene]-5,6-dihydro-6-imino-1,3-dimethyluracil which was refluxed with thiourea in EtOH contg. NaOEt to give 52% I (R1 = R2 = Me, R3 = H, R4 = NH₂) (II). In rats 20 mg II/kg orally gave 53.3% inhibition of passive cutaneous anaphylaxis reaction compared to 67.3% for theophylline.

IT **56007-62-6P 94839-44-8P 94839-45-9P**

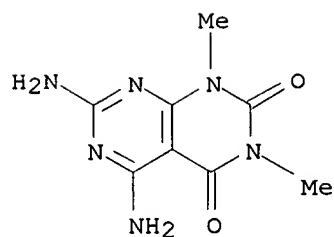
101989-67-7P 101989-73-5P 101989-74-6P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of, as allergy inhibitor)

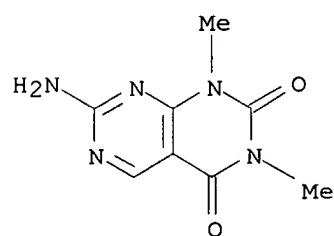
RN 56007-62-6 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 5,7-diamino-1,3-dimethyl- (9CI) (CA INDEX NAME)



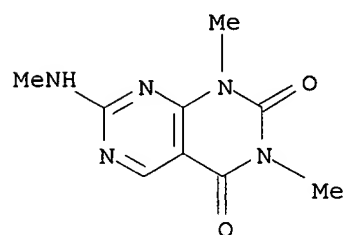
RN 94839-44-8 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-1,3-dimethyl- (9CI)
(CA INDEX NAME)



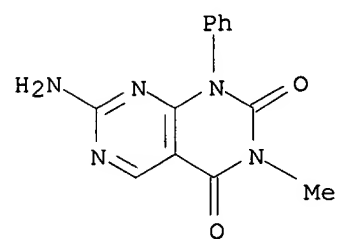
RN 94839-45-9 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 1,3-dimethyl-7-(methylamino)-
(9CI) (CA INDEX NAME)

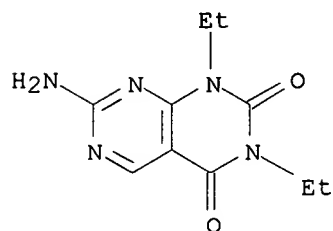


RN 101989-67-7 CAPLUS

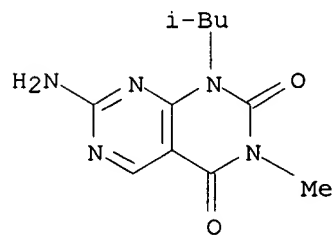
CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-3-methyl-1-phenyl-
(9CI) (CA INDEX NAME)



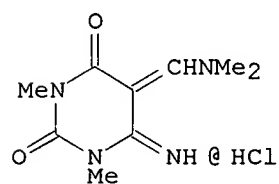
RN 101989-73-5 CAPLUS
 CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-1,3-diethyl- (9CI)
 (CA INDEX NAME)



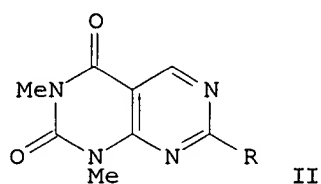
RN 101989-74-6 CAPLUS
 CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-3-methyl-1-(2-methylpropyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1985:95601 CAPLUS
 DOCUMENT NUMBER: 102:95601
 TITLE: A facile synthesis of 7-substituted
 pyrimido[4,5-d]pyrimidine-2,4-diones
 AUTHOR(S): Hirota, Kosaku; Kitade, Yukio; Sajiki, Hironao; Maki,
 Yoshifumi
 CORPORATE SOURCE: Gifu Pharm. Univ., Gifu, 502, Japan
 SOURCE: Synthesis (1984), (7), 589-90
 CODEN: SYNTBF; ISSN: 0039-7881
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



I



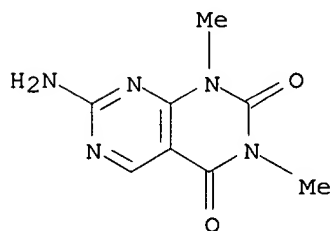
II

AB Cyclization of uracil I with RC(X)NH₂ (R = H, Me, CF₃, Ph, H₂N, MeNH; X = O, S, NH) gave 52-92% 7 title compds. II.

IT **94839-44-8P 94839-45-9P**
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and spectra of)

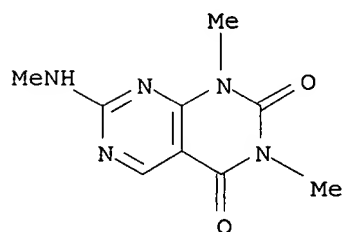
RN 94839-44-8 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-1,3-dimethyl- (9CI)
 (CA INDEX NAME)



RN 94839-45-9 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 1,3-dimethyl-7-(methylamino)-
 (9CI) (CA INDEX NAME)



L4 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1981:156846 CAPLUS

DOCUMENT NUMBER: 94:156846

TITLE: Phosgeniminium salts. Part 28. Annulation of 5 or 6
 membered heterocycles to uracil derivatives via
 phosgeniminium salt condensation

AUTHOR(S): Kokel, B.; Lespagnol, C.; Viehe, H. G.

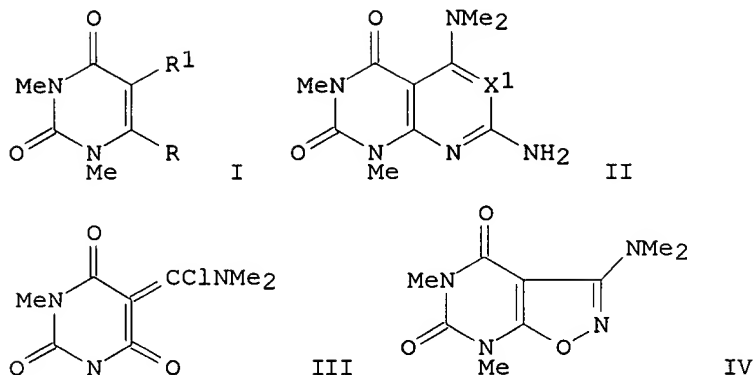
CORPORATE SOURCE: Lab. Chim. Org., Univ. Louvain, Louvain-la-Neuve,
 B-1348, Belg.

SOURCE: Bull. Soc. Chim. Belg. (1980), 89(8), 651-7
 CODEN: BSCBAG; ISSN: 0037-9646

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



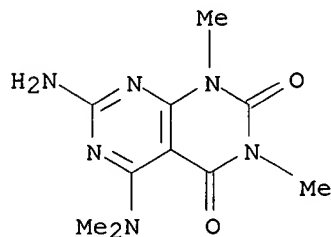
AB Reaction of the uracil I (R = NH₂, R₁ = H) with Me₂N⁺:CCl₂Cl⁻ gave I (R = NH₂, R₁ = CCl₂NMe₂) which reacted with nucleophiles to give I [R = NH₂, R₁ = CXNMe₂, X = O, NPh, NNH₂, NCN, C(CN)₂]. The latter 2 compds. were hydrolyzed to II (X₁ = N, CCN). Reaction of, I (R = OH, R₁ = H) with Me₂N⁺:CCl₂Cl⁻ gave III which also reacted with nucleophiles to give I (R = OH, R₁ = CXNMe₂, X = NH, NPh, NOH). The latter compd. was cyclized by heating to IV.

IT 77008-19-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 77008-19-6 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione,
7-amino-5-(dimethylamino)-1,3-
dimethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1976:74208 CAPLUS

DOCUMENT NUMBER: 84:74208

TITLE: Cycloacylation of enamines. III. Synthesis and reactions of pyrimido[4,5-d]pyrimidines

AUTHOR(S): Grohe, Klaus; Heitzer, Helmut

CORPORATE SOURCE: Zent. Forsch., Bayer A.-G., Leverkusen, Ger.

SOURCE: Justus Liebigs Ann. Chem. (1975), Volume Date 1974, (12), 2066-73

CODEN: JLACBF

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB Reaction of the 4-aminouracils I with Cl₃CN:CCl₂, Cl₃CCCl:NCCl₂CCl₃, PhCCl₂N:CCl₂, or Cl₃CCCl₂NCO gave by cycloacylation the pyrimidopyrimidines II (R = Me, CH₂CH₂Ph, CH₂:CHCH₂, or H; R₁ = Me, R₂ = CCl₃, R₃ = Cl), II (R = R₁ = Me, R₂ = Cl, R₃ = Ph) and II (R = R₁ = Me,

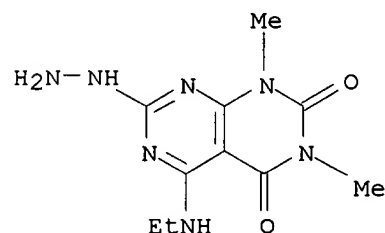
R₂ = Ph, R₃ = Cl), or II (R = R₁ = Me, R₂ = CCl₃, R₃ = OH), resp. Some nucleophilic substitution reactions of III were reported.

IT **56007-74-0P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and reaction with nitrofuraldehyde)

RN 56007-74-0 CAPLUS

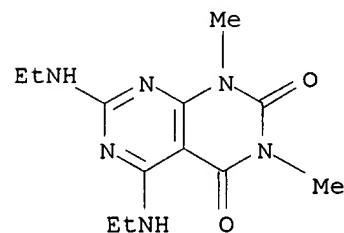
CN Pyrimido[4,5-d]pyrimidine-2,4,7(1H,3H,6H)-trione, 5-(ethylamino)-1,3-dimethyl-, 7-hydrazone (9CI) (CA INDEX NAME)

IT **56007-61-5P 56007-62-6P 56007-63-7P****56007-64-8P 56007-65-9P 56007-66-0P****56007-71-7P 56007-75-1P**

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

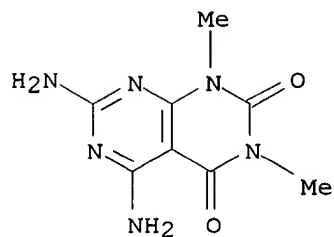
RN 56007-61-5 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 5,7-bis(ethylamino)-1,3-dimethyl- (9CI) (CA INDEX NAME)



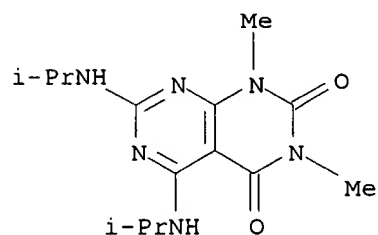
RN 56007-62-6 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 5,7-diamino-1,3-dimethyl- (9CI) (CA INDEX NAME)



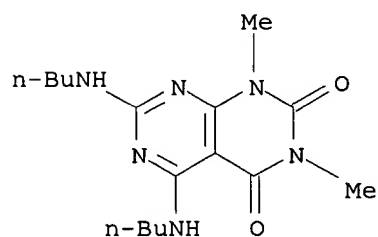
RN 56007-63-7 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 1,3-dimethyl-5,7-bis[(1-methylethyl)amino]- (9CI) (CA INDEX NAME)



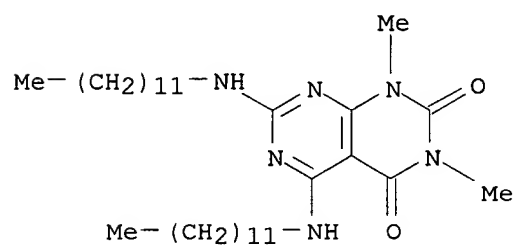
RN 56007-64-8 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 5,7-bis(butylamino)-1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 56007-65-9 CAPLUS

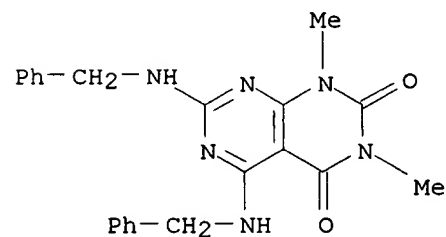
CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 5,7-bis(dodecylamino)-1,3-dimethyl- (9CI) (CA INDEX NAME)



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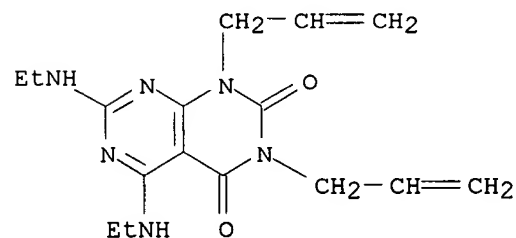
RN 56007-66-0 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 1,3-dimethyl-5,7-bis[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



RN 56007-71-7 CAPLUS

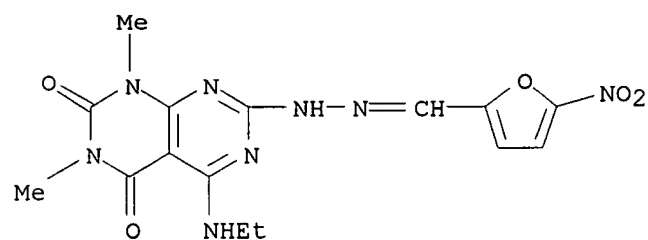
CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 5,7-bis(ethylamino)-1,3-di-2-propenyl- (9CI) (CA INDEX NAME)



RN 56007-75-1 CAPLUS

CN 2-Furancarboxaldehyde, 5-nitro-, [4-(ethylamino)-5,6,7,8-tetrahydro-6,8-dimethyl-5,7-dioxypyrimido[4,5-d]pyrimidin-2-yl]hydrazone (9CI) (CA

INDEX
NAME)



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(FILE 'HOME' ENTERED AT 09:11:18 ON 09 FEB 2000)

FILE 'REGISTRY' ENTERED AT 09:11:26 ON 09 FEB 2000

L1 STRUCTURE UPLOADED

09/ 422,451

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L3 72 S L1 FUL

FILE 'CAPLUS' ENTERED AT 09:12:09 ON 09 FEB 2000
L4 10 S L3

=> log y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	40.22	166.67
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-5.57	-5.57

STN INTERNATIONAL LOGOFF AT 09:13:24 ON 09 FEB 2000